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Dynamics of Condensate Shells: Collective Modes and Expansion

Courtney Lannert
Wellesley College, clannert@smith.edu

T. C. Wei
University of Illinois Urbana-Champaign

S. Vishveshwara
University of Illinois Urbana-Champaign

Dynamics of condensate shells: Collective modes and expansion

C. Lannert,[1] T.-C. Wei,[2] and S. Vishveshwara[2]
[1]*Wellesley College, Wellesley, Massachusetts 02481, USA*
[2]*University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA*
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We explore the physics of three-dimensional shell-shaped condensates, relevant to cold atoms in "bubble traps." We study the ground state of the condensate wave function, spherically symmetric collective modes, and expansion properties of such a shell using a combination of analytical and numerical techniques. We find two breathing-type modes with frequencies that are distinct from that of the filled spherical condensate. Upon trap release and subsequent expansion, we find that the system displays self-interference fringes. We estimate characteristic time scales, degree of mass accumulation, three-body loss, and kinetic energy release during expansion for a typical system of ^{87}Rb.

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The cooling and trapping of dilute atoms has recently achieved unprecedented levels of control and sophistication. With the advent of optical lattices [1], quasi-one- and quasi-two-dimensional trapping potentials [2], and mixtures of different species [3], condensates of bosonic atoms have been created in a plethora of interesting geometries. Boson mixtures in a particular regime of interactions can form a layered or core-and-shell structure [4]. Bosons in a three-dimensional optical lattice also display a shell structure as a result of the confining trap [5]. It may even be possible to confine a dilute atomic condensate to a spherical shell-shaped region by means of a specifically designed "bubble trap" [6]. Towards an understanding of these, and other systems where superfluid order exists in "hollow" geometries, we consider the physics of a condensate whose shape is a three-dimensional spherical shell. We identify key features in the condensate collective modes and expansion upon trap release that distinguish such shell-shaped condensates from the more common filled cases. Moreover, we find that expansion properties have distinct similarities with "Bose-nova" experiments [7].

A condensate confined by a three-dimensional confining potential of the form $V(\mathbf{r})=(1/2)m\omega_0^2(r-r_0)^2$ (where m is the atomic mass) at zero temperature and weak interatomic interaction obeys the time-independent Gross-Pitaevskii (GP) equation:

$$\left(-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r})+g|\psi(\mathbf{r})|^2\right)\psi(\mathbf{r})\equiv\frac{\delta\mathcal{H}}{\delta\psi^*}=\mu\psi(\mathbf{r}),\quad(1)$$

where g is a measure of the repulsive interactions between the atoms ($g=4\pi\hbar^2a/m$ with a the s-wave scattering length) and μ is the chemical potential, set by the normalization condition: $\int|\psi(\mathbf{r})|^2d^3r=N$. The density of condensed atoms is given by $n(\mathbf{r})=|\psi(\mathbf{r})|^2$.

For suitably large N, the kinetic energy is very small compared to the potential energies and the gradient term may be neglected (the Thomas-Fermi approximation) [8], giving an approximate ground state wave function $\psi_{\mathrm{TF}}(\mathbf{r})=\sqrt{[\mu-V(\mathbf{r})]/g}$ in the regions where $\mu\geqslant V(\mathbf{r})$ and zero elsewhere. In this approximation, the condensate occupies a spherically symmetric shell centered at r_0 with half-width $r_1=\sqrt{2\mu/(m\omega_0^2)}$. In the limit of a thin shell ($r_1\ll r_0$), r_1 is found to be $[3gN/(8\pi m\omega_0^2r_0^2)]^{1/3}$. Therefore, for the Thomas-Fermi wave function, the condition for a thin shell can be written

$$\Gamma_{ts}\equiv\frac{r_1}{r_0}=\left(\frac{3gN}{8\pi m\omega_0^2r_0^5}\right)^{1/3}=\left(\frac{3Na_{\mathrm{osc}}a}{2r_0^5}\right)^{1/3}\ll1,$$

where we have introduced the oscillator length $a_{\mathrm{osc}}\equiv\sqrt{\hbar/(m\omega_0)}$. In order to obtain analytic results, we will often work within this "thin shell" limit. While applicable to typical conditions in bubble traps and optical lattice systems, we also expect an analysis of thin shells to capture the salient features of thicker shells. Notable expected differences will be discussed in some cases.

While we are able to go beyond the Thomas-Fermi approximation using numerical techniques, it is worth estimating its regime of validity. Using a radially symmetric Gaussian wave function centered at radius R_0 and with characteristic width R_1, we find the ratio of the zero-point kinetic energy to the potential energy of interaction to scale as $R_0^2/(NaR_1)$. [The analogous ratio for a condensate in a harmonic trap centered at $r=0$ scales as $R/(Na)$ (see, e.g., Ref. [4])]. Hence, for the shell (i.e., taking R_0 to be r_0 and R_1 to be r_1), the Thomas-Fermi approximation can be expected to be valid when $\Gamma_{\mathrm{TF}}\equiv r_0^2/(Nar_1)=[(2r_0^8)/(3N^4a_{\mathrm{osc}}^4a^4)]^{1/3}\ll1$.

For a trap with $\omega_0=2\pi\times20$ Hz and $r_0=20a_{\mathrm{osc}}$ and a cloud of $N=10^6$ atoms of ^{87}Rb in the $|F=1,m_F=-1\rangle$ or $|F=2,m_F=2\rangle$ state (for which $a\approx5.45$ nm [9]), we have $\Gamma_{ts}=r_1/r_0\approx0.08$ and $\Gamma_{\mathrm{TF}}\approx0.09$. In excellent numerical agreement, using the imaginary time technique of Chiofalo *et al.* [10] and the parameters given above, we find the ratio of the kinetic energy to the total energy in the ground state to be $K/E_{\mathrm{tot}}\simeq0.093$.

Towards obtaining the lowest-energy collective modes of a thin spherical shell of superfluid, we consider a trial wave function for the shell condensate of the form

$$\psi_{\mathrm{trial}}[R_0,R_1]=\mathcal{A}\frac{\sqrt{N}}{R_0\sqrt{R_1}}\mathcal{F}\left(\frac{r-R_0}{R_1}\right)e^{i\phi(\mathbf{r})},\quad(2)$$

where $\mathcal{A}$ is a dimensionless normalization constant (in the thin shell limit) and $\mathcal{F}$ is a smooth real function that is negligibly small for $|r-R_0|\gg R_1$ [for instance a Gaussian, $\mathcal{F}(x)=e^{-x^2/2}$]. We note that except for the discontinuity at the condensate boundary, the Thomas-Fermi wave function is in the class of wave functions described by Eq. (2). The function $\phi(\mathbf{r})$ has the usual relation to the velocity of the condensate, $\mathbf{v}=\hbar\boldsymbol{\nabla}\phi/m$. R_0 and R_1 are variational parameters corresponding to the average radius and characteristic width of the cloud, respectively. A description of the cloud in terms of the collective coordinates R_0 and R_1 is expected to capture the salient features of the isotropic, $\ell=0$, collective modes of the superfluid shell.

Collective modes. Starting with the variational wave function in Eq. (2) and allowing the parameters R_0 and R_1 to vary in time, standard methods yield equations of motion for these collective coordinates (see, e.g., Ref. [4]). We start by noting that the energy of the condensate for a wave function of the form Eq. (2) can be written as

$$\mathcal{H}[R_0,R_1,\phi]=\frac{m}{2}\int n(\mathbf{r})|\mathbf{v}(\mathbf{r})|^2d^3r+\mathcal{U}_{\text{eff}}, \tag{3}$$

where $\mathcal{U}_{\text{eff}}$ is equal to the energy of the cloud if the phase ϕ does not vary in space and acts as an effective potential for the collective coordinates R_0 and R_1. It can be written in a physically transparent form as a sum of contributions from zero-point (or confinement) energy, potential energy from the trap, and interaction energy, $\mathcal{U}_{\text{eff}}[R_0,R_1]=E_{\text{zp}}+E_{\text{tr}}+E_{\text{int}}$. When the system is in equilibrium, $\mathbf{v}(\mathbf{r})=0$ and minimization of Eq. (3) yields the variational ground state values of R_0 and R_1. For the trial wave function in Eq. (2), in the thin shell limit $(R_1\ll R_0)$, we find

$$E_{\text{zp}}=\frac{\hbar^2}{2m}\int\left(\frac{d|\psi|}{dr}\right)^2d^3r\approx\frac{c_{\text{zp}}}{R_1^2},$$

$$E_{\text{tr}}=\int V(\mathbf{r})|\psi|^2d^3r\approx\frac{Nm}{2}\omega_0^2[c_{\text{tr}}R_1^2+(R_0-r_0)^2],$$

$$E_{\text{int}}=\frac{g}{2}\int|\psi|^4d^3r\approx\frac{c_{\text{int}}}{R_0^2R_1},$$

to lowest nonvanishing order in R_1/R_0, where c_{zp}, c_{tr}, and c_{int} are independent of R_0 and R_1 and are determined by the form of the function $\mathcal{F}$ in Eq. (2).

The variational energy, Eq. (3) can be used to find two, low-energy, collective excitations of the superfluid shell: one in which the width, R_1, oscillates around its equilibrium value (the "accordion mode") and another in which the average radius of the cloud, R_0, oscillates around its equilibrium value, r_0 (the "balloon mode"). For simplicity, we assume that in the accordion mode, the mean radius of the shell stays fixed at r_0 while the width oscillates and that in the balloon mode the width, R_1, remains fixed while the mean radius oscillates. While it is clear that any exact solution will couple changes in the width to changes in the mean radius, the "decoupled" oscillations we consider here can be expected to illuminate the correct low-energy physics. Indeed, in the thin shell limit, we find that oscillations in R_1 do not affect the mean radius R_0 and that oscillations in R_0 affect the width, R_1, at a negligible level for small oscillations about equilibrium [smaller by a factor $(R_0-r_0)/r_0$].

The balloon mode. For this mode, we consider a velocity field of the form $\mathbf{v}_b=\beta\hat{\mathbf{r}}$, where $\beta[r,\dot{R}_0,\dot{R}_1]$ is a variational parameter, or equivalently, $\phi(\mathbf{r})=\beta mr/\hbar$. As a lowest-order approximation, we hold R_1 fixed at its equilibrium value, r_1, and only allow R_0 to vary in time. By constructing a Lagrangian for the parameters R_0 and β, we find $\beta=\dot{R}_0\Rightarrow\mathbf{v}_b=\dot{R}_0\hat{r}$ and an equation of motion for R_0,

$$mN\ddot{R}_0=-\frac{\partial\mathcal{U}_{\text{eff}}}{\partial R_0}=\frac{2c_{\text{int}}}{R_0^3r_1}-Nm\omega_0^2(R_0-r_0). \tag{4}$$

In the thin shell limit, Eq. (4) yields $R_0^{\text{eq}}=r_0$ and a frequency of small oscillations around this equilibrium value

$$\omega_b\simeq\omega_0+O(r_1^2/R_0^2). \tag{5}$$

We note that the thin-shell approximation imposes a constraint on the amplitude of oscillations in R_0, $R_0^{\text{min}}\gg r_1$.

The accordion mode. For this mode, we consider a velocity field for the condensate of the form $\mathbf{v}_a=\beta(r-r_0)\hat{\mathbf{r}}$ [equivalently, $\phi(\mathbf{r})=\beta m(r-r_0)^2/(2\hbar)$] and allow R_1 to vary in time while holding R_0 fixed at its equilibrium value, r_0. Following the same procedure as for the balloon mode, we find $\beta=\dot{R}_1/R_1\Rightarrow\mathbf{v}_a=\hat{\mathbf{r}}(r-r_0)R_1/R_1$ and an equation of motion for R_1,

$$m_{\text{eff}}^a\ddot{R}_1=-\frac{\partial\mathcal{U}_{\text{eff}}}{\partial R_1}=\frac{2c_{\text{zp}}}{R_1^3}+\frac{c_{\text{int}}}{R_1^2r_0^2}-m_{\text{eff}}^a\omega_0^2R_1, \tag{6}$$

with $m_{\text{eff}}^a\equiv4\pi m\mathcal{A}^2N\int_{-\infty}^{\infty}q^2\mathcal{F}^2(q)dq$. Using the fact that $\partial\mathcal{U}_{\text{eff}}/\partial R_1=0$ at equilibrium, the frequency of small oscillations of R_1 about its equilibrium value can be written

$$\omega_a=\omega_0\sqrt{4-\frac{E_{\text{int}}}{2E_{\text{tr}}}}. \tag{7}$$

The thin-shell approximation imposes a constraint on the amplitude of oscillations in R_1, $R_1^{\text{max}}\ll r_0$. In the limit of weak interactions, $E_{\text{int}}\ll E_{\text{tr}}$, Eq. (7) reduces to $\omega_a=2\omega_0$. Thus, in the weak interaction limit, the frequency of this mode is equivalent to that of the breathing mode of a spherical condensate cloud. In the limit of strong interactions, $E_{\text{int}}\gg E_{\text{zp}}$, we have $E_{\text{int}}\simeq2E_{\text{tr}}$ and find $\omega_a=\sqrt{3}\omega_0$. This result should be compared with the strong interaction limit of the spherical breathing mode, $\omega_{br}=\sqrt{5}\omega_0$.

We note that the modes in the thin-shell limit described by Eq. (5) and Eq. (7) have a structure identical to that of a one-dimensional condensate, corresponding to its one-dimensional sloshing and breathing modes, respectively [11]. For thicker shells, we expect corrections to our results that couple the R_1 and R_0 degrees of freedom. In fact, in the limit that $R_0\to0$ we expect the balloon and accordion modes to tend to the breathing mode and next radially symmetric mode $(n=2)$ of a filled spherical condensate with $R_0=0$.

Expansion. The dynamics of the spherical shell upon release of the trapping potential has noteworthy features absent in the case of the filled sphere. Upon release, the initial confinement of the condensate causes the outer edge to expand outwards and the inner edge to collapse inwards. As a result, the system can potentially exhibit accumulation of mass at the center, and the condensate can interfere with itself when diametrically opposite regions come together.

The time scale of expansion can be estimated within the thin-shell approximation (where the dynamics of the width, R_1, do not affect the mean radius, R_0, which we approximate as fixed at r_0). Taking the function $\mathcal{F}$ in Eq. (2) to be a Gaussian and evaluating the different energy contributions as before, we find that energy conservation between the instant the trap is switched off and later times t gives the relationship

$$\frac{\hbar^2}{mR_1^2(0)}+\frac{gN}{(2\pi)^{3/2}R_1(0)r_0^2}=m\dot{R}_1^2+\frac{\hbar^2}{mR_1^2}+\frac{gN}{(2\pi)^{3/2}R_1r_0^2},$$

where the time argument of $R_1(t)$ on the right-hand side is suppressed, and $R_1(0)$ is the characteristic width of the condensate shell before expansion. Assuming the initial energy is dominated by the interaction energy, we find that, on the time scale for which the shell expands enough to become dilute but not enough to reach the center, $R_1^2(t)/R_1^2(0) \approx 2\omega_0^2t^2$, in contrast to a filled sphere for which $R_1^2(t)/R_1^2(0)\approx(2/3)\omega_0^2t^2$ [4]. Hence, for typical parameters used in this paper, a shell of initial thickness 5 μm and radius 50 μm should expand to a thickness of $R_1(t)=20$ μm on a time scale of around 20 ms, which is amenable to experimental detection.

To quantify the physics of the expanding shell, we performed a numerical time evolution of the initial condensate wave function (given by the numerically obtained result discussed earlier) after release from the trap, including interactions. This expansion process was obtained using the real-time synchronous Visscher method [12] to integrate the time-dependent GP equation, $i\hbar d\psi/dt=\delta\mathcal{H}/\delta\psi^*$. The results are shown in Fig. 1.

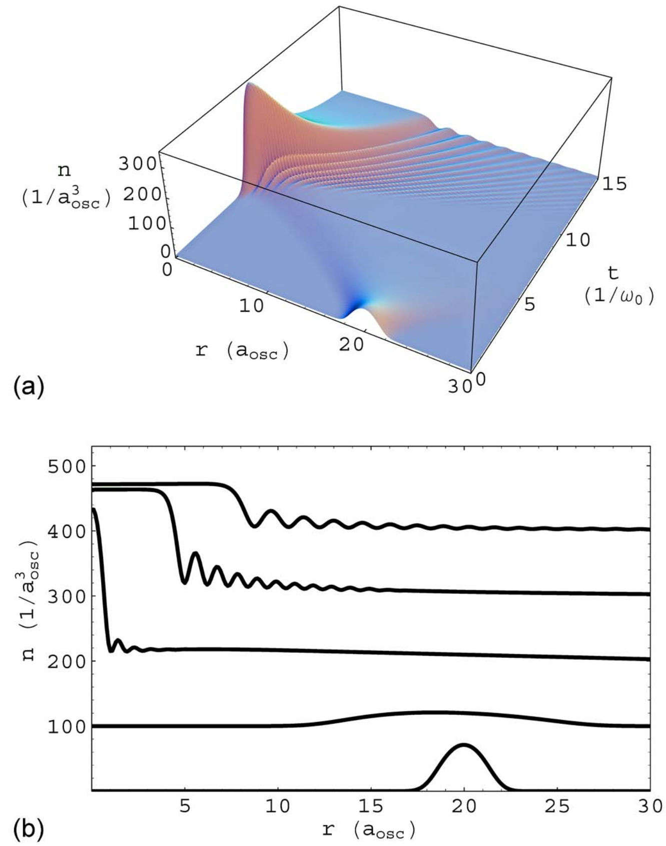

FIG. 1. (Color online) Expansion of a thin spherical shell. (a) Evolution of the density as a function of radial position and time. (b) Snapshots of the density profile at times $t=0,3,6,9,12$ (from the lowest curve, subsequent curves are shifted up by 100 for clarity).

Two general features of the expansion deserve discussion. First, mass accumulation in the center can result in a density greater (but not necessarily much greater) than the initial density. We note that repulsive interactions between the atoms prevent the density from becoming as large as it would in the noninteracting case. Second, interference fringes appear after the inner radius of the cloud has reached the origin, demonstrating self-interference of the condensate. For two Gaussian condensates initially separated by a distance D, the fringe size at long times is given by $\delta_r=2\pi\hbar t/(mD)$ [4] in the absence of interactions. The free expansion of an initially thin Gaussian shell is straightforward to calculate and we find that the fringe spacing at long times is identical to that of two Gaussian condensates, but with the initial separation, D, replaced by the initial diameter of the shell, $2r_0$. This implies $\delta_r=\pi t\omega_0 a_{\rm osc}^2/r_0$, which for $r_0=20a_{\rm osc}$ gives a fringe spacing at time $t\omega_0=10$ of $\delta_r\simeq 1.6a_{\rm osc}$. This compares to an average fringe size observed in our numerics of about $1.2a_{\rm osc}$. The difference in precise values presumably results from the effects of interparticle interactions and the non-Gaussian shape of the initial wave function.

The dynamics of the shell upon trap release has distinct parallels with the Bose-nova collapse of a condensate when the interatomic interactions are switched from repulsive to attractive. For the shell, the initial implosion is caused by the quantum pressure of the condensate forcing itself to fill the low-density region at the center. Similar to the Bose-nova case, mass buildup near the origin is followed by a relaxation and expansion on time scales comparable to the trap frequency. An important question, given these parallels, is whether three-body recombination and subsequent "loss" of atoms is appreciable in the case of the released shell (as it is in the case of the Bose-nova collapse [7]). These losses are described by the equation $dn/dt=-K_3n^3$ where K_3 is the three-body loss rate [4]. Concentrating on the time in our numerics with the largest density (at $t\approx 6.5/\omega_0$), we estimate that the density in the central plateau is $n\simeq 350/a_{\rm osc}^3$ over a radius of about $a_{\rm osc}$. Assuming that this density persists for the entire time between snapshots, $\delta t\approx 3/\omega_0$, and taking $K_3=4.0\times10^{-30}$ cm^6/s [4], we find an upper bound on the number of particles lost in this region during this time slice of $\Delta N\simeq 0.09$, making three-body recombination negligible for the case considered here.

The effects of mass accumulation would be enhanced if only the inner edge of the trap were removed, suppressing the outward expansion of the condensate. This more dramatic case was considered by Zobay and Garraway [6], in which they modeled an initially shell-shaped trap quickly switched into a harmonic trap. Similar features of mass accumulation and self-interference fringes were found in the case of this bubble trap. For a shell with the parameters given in this paper, we can estimate the time scale for collapse and the kinetic energy gain in this scenario by considering a small cavity of radius R_2 at the center of a condensate. In the Thomas-Fermi approximation, the dynamics of such a cavity can be mapped to the standard hydrodynamics problem of a collapsing bubble in a fluid governed by the equation [13]

$$\frac{p-p_0}{\rho}=\frac{R_2^2\ddot{R}_2+2R_2\dot{R}_2{}^2}{r}-\frac{R_2^4\dot{R}^2}{2r^4}. \tag{8}$$

Here, $\rho=mn$ is the condensate mass density, p is the pressure at radius r and $p_0=n^2g/2$ is the pressure far from the cavity. Integrating Eq. (8) at the edge of the bubble $(r=R_2)$ and making the substitution $R_2(t)=R_2(0)x^{1/3}$ gives the time for complete collapse in terms of the initial radius, $R_2(0)$: $t_f \approx 0.915R_2(0)\sqrt{\rho/p_0}$. The kinetic energy gained by the particles upon reaching the center is given by $E_{\mathrm{KE}} = 4\pi/3p_0R_2^3(0)$. For a cavity of radius 40 μm and quantum pressure of magnitude $p_0=1\times10^{-14}$ erg/cm^3, the collapse time is on the order of 100 ms and the kinetic energy gained per particle is on the order of 1 nK. The small cavity treatment suggests that the collapse of the inner radius can be accompanied by a measurable amount of kinetic energy gain and mass accumulation.

In conclusion, motivated by possible new trapping potentials for dilute ultracold atoms, as well as general interest in new geometries for Bose-Einstein condensates, we have explored the collective modes and expansion dynamics of a superfluid confined to a spherical shell. The two breathing modes we find are distinct from those of a filled spherical condensate in the limit of strong interactions. The expansion properties of the shell after release from the trap are found to have some notable similarities with Bose-nova physics, particularly mass accumulation and self-interference.

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